

Phenol, 4-chloro-2-methoxy-
16766-30-6 | DTXSID0074974

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.90e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.28e-01

Confidence level: 4.89e-01

Nearest Neighbors from the Training Set

Image not found

1,6-Naphthyridin-8-ol

Measured: 2.20e-02

Predicted: 5.00e-02

Image not found

2,2,2-Trichloroethanol

Measured: 5.58e-01

Predicted: 5.36e-01

Image not found

Ethanol, 2-(phenylamino)-

Measured: 3.35e-01

Predicted: 8.15e-01